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An Alternative Approach to Quantum Statistics

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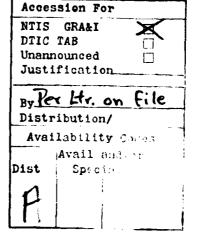Naval Research Laboratory, Washington, D.C. 20375

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Abstract

The Fermi-Dirac, Bose-Einstein and, for completeness the Maxwell-Boltzmann, distributions are obtained respectively from considerations of binomial, negative binomial, and Poisson assemblies. The method used has the simplicity of the traditional derivations that are based on combinatorial considerations but involves neither the identification of most probable values with mean values nor the invocation of large numbers of particles involved in the use of Stirling's approximation for factorials. The method thereby also relaxes the requirement for large numbers of particles needed in other available derivations that also use mean values, namely, the Darwin-Fowler method of steepest descents and the Khinchin method that employs limit theorems of the theory of probability.

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I. Introduction

Although quantum statistics have been consistently verified empirically in the approximately sixty years since their introduction, there remain disquieting aspects about the way in which Fermi-Dirac and Bose-Einstein occupation factors are derived. The most straightfoward way[1] to derive these occupation factors uses combinatorial methods to enumerate distinguishable arrangements for indistinguishable particles described respectively by antisymmetric wave functions for Fermi-Dirac statistics, and symmetric wave functions for Bose-Einstein statistics. With the enumeration in hand and factorials expressed in the Stirling's approximation, an extremum principle subject to appropriate constraints on total number of particles and total energy is used to yield the most probable distribution of particles. This most probable distribution is considered equivalent to the mean value distribution which is in turn directly related to the desired occupation factor.

Although the difference between the most probable distribution and the mean value distribution is not great, dissatisfaction with the use of this mathematical approximation in the derivation of the fundamental quantum statistical distributions has led to alternative, more complicated but rigorous, derivations based on mean values. These alternative derivations include the Darwin-Fowler method of steepest descents,[2] and Khinchin's use of limit theorems of the theory of probability.[3] However, even these derivations share with the combinatorial approach the requirement that the total number of particles under consideration be very large. Since quantum statistics applies even for small total number of particles, it is desirable to develop a derivation that both uses mean values and relaxes the requirement that the total number of particles under consideration be very large. This is indeed the object of the present paper.

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The new approach used here has the simplicity of the combinatorial method but deals directly with mean values and does not require the approximation of a large total number of particles. The starting point is the use of Bernoulli trials and related probability distributions, namely the binomial, negative binomial, and Poisson distributions. Assemblies of such distributions are used respectively to derive the Fermi-Dirac (sec. II), Bose-Einstein (sec. III), and Maxwell-Boltzmann (sec. IV) occupation factors by application of an entropy extremum principle. The entropy extremum principle is closely related to one recently used by Grandy[4] to derive the various occupation factors. An important distinction between Grandy's approach and the present one is the basis for the definition of entropy.

The present approach shares with its predecessors an apparent requirement that the particles are non-interacting, i.e., that many particle quantities are built up from one particle entities. This seems paradoxical since the *relative particle occupancies should be based on some* sort of coupling among the particles either directly or through a thermal reservoir. In fact the assumption of non-interacting particles may be understood to mean that a one-particle basis is valid at thermal equilibrium in that all interactions are subsumed into the manner in which constraint conditions are introduced. From that viewpoint, the assumption of non-interacting particles is appropriate for the derivation of occupation factors for particles.

After the various occupation probabilities are derived in the next three sections, concluding remarks are made in section V.

II. Binomial Assemblies and Fermi-Dirac Statistics

A binomial assembly consists of all possible binomial distributions generated in the expansion of

$$(p+q)^R = 1 \tag{2.1}$$

where R is the number of trials, p is the probability of success in a trial, and q=1-p is the probability of failure. A typical term, say the Nth term provides the binomial probability (frequency) function for N successes in R trials.

$$F_R(N,p) = \binom{R}{N} p^N q^{R-N} \tag{2.2}$$

The mean value for the number of successful trials is

$$\langle N \rangle = \sum_{N=0}^{R} N \, F_R(N,p) = p \frac{\partial}{\partial p} (p+q)^R = Rp \tag{2.3}$$

If the number of trials, R, is identified as the number of possible occupations or cells, and the mean number of successes, $\langle N \rangle$, is identified as the mean number of occupations, then p may be identified as the occupation factor. In this way the language of the binomial distribution is translated into the language of particle statistics.

First observe that indeed the combinatorial factor on the right hand side of Eq. (2.2), $\binom{R}{N}$, *provides the number of distinguishable ways of achieving N occupations in R cells when the exclusion principle (the occupation number for individual cells may be 0 or 1) applies.* Thus contact is immediately established with the concepts usually involved in Fermi-Dirac statistics. The combinatorial factor will be designed the weight function

$$W_R(N) \equiv \binom{R}{N} = \frac{R!}{N!(R-N)!} \tag{2.4}$$

The remaining factor in the right hand side of Eq. (2.2) will be designated the load function,

$$\Lambda_R(N,p) \equiv p^N q^{R-N} \tag{2.5}$$

Equation (2.2) then takes the form,

$$F_R(N,p) = W_R(N) \, \Lambda_R(N,p) \tag{2.6}$$

It is important to note that the mean number of occupations $\langle N \rangle$ is computed with the help of the complete $F_R(N,p)$. Given this $\langle N \rangle$ and Eq. (2.3), $\ell n \Lambda_R(\langle N \rangle, p)$ may be expressed in the form

$$\ell n \Lambda_R(\langle N \rangle, p) = R[p\ell np + (1-p)\ell n(1-p)] \equiv -RS(p)/k \tag{2.7}$$

Here $S(p) \equiv -k[p\ell np + (1-p)\ell n(1-p)]$ is the Shannon entropy[5,6] of the occupation factor p, where k is the Boltzmann constant.

Consider now a set of J binomial assemblies each labelled by an index j corresponding to physical levels. The assemblies will be considered non-interacting so that any coupling that influences their relative occupations is subsumed into subsidiary constraint conditions. Then the possible distributions for the set are generated by the product of all possible distributions for the individual assemblies:

$$\prod_{j=1}^{J} \{p(j) + q(j)\}^{R(j)} = 1 \qquad . \tag{2.8}$$

A typical distribution may be characterized by a set of numbers of occupations within the individual assemblies

$$\underset{\sim}{N} = [N(1), N(2), \ldots, N(J)] \tag{2.9}$$

for the complete set of occupation possibilities (cells),

$$\underset{\sim}{R} = [R(1), R(2), \ldots, R(J)] \qquad . \tag{2.10}$$

The probability for $\underset{\sim}{N}$ occupations in $\underset{\sim}{R}$ cells is then

$$F_{\underset{\sim}{R}}(\underset{\sim}{N}, \underset{\sim}{p}) = \prod_{j=1}^{J} W_{R(j)}(N(j))\Lambda_{R(j)}(N(j), p(j)) \tag{2.11}$$

where

$$\underset{\sim}{p} \equiv [p(1), p(2), \ldots, p(J)] \tag{2.12}$$

Equation (2.11) may be written in the form

$$F_{\underset{\sim}{R}}(\underset{\sim}{N}, \underset{\sim}{p}) = W_{\underset{\sim}{R}}(\underset{\sim}{N})\Lambda_{\underset{\sim}{R}}(\underset{\sim}{N}(\underset{\sim}{N}, \underset{\sim}{p}) \qquad , \tag{2.13}$$

where

$$W_R(\underset{\sim}{N}) \equiv \prod_{j=1}^{J} W_{R(j)}(N(j)) \tag{2.14}$$

and

$$\Lambda_{\underset{\sim}{R}}(\underset{\sim}{N},\underset{\sim}{p}) \equiv \prod_{j=1}^{J} \Lambda_{(R(j)}(N(j),p(j)) \quad . \tag{2.15}$$

In the traditional combinatorial treatment[1] of Fermi-Dirac statistics, $\ell n W_{R}(\underset{\sim}{N})$ is expressed in Stirling's approximation and, subject to subsidiary conditions, maximized with respect to $N(j)$. The maximization is carried out by the method of Lagrange undetermined multipliers into which the particles' interaction with a heat reservoir are subsumed. The eventual result is the most probable value of $N(j)$. No attention is paid to the load function in this traditional approach. $\ell n W_{R}(\underset{\sim}{N})$ is related to the entropy so that this procedure is an entropy maximum principle.

The emphasis in the present treatment is on the mean number of occupations, i.e., $\langle N(j) \rangle$ or equivalently, by Eq. (2.3), the occupation factors $p(j)$. A traditional _minimization_ principle is applied to the function $\ell n \Lambda_{R}(\langle \underset{\sim}{N} \rangle, \underset{\sim}{p})$ subject to subsidiary conditions, by variation with respect to $p(j)$. Note that

$$\ell n \Lambda_{\underset{\sim}{R}}(\langle \underset{\sim}{N} \rangle,\underset{\sim}{p}) = \sum_{j=1}^{J} R(j)\{p(j)\ell n p(j)+[1-p(j)]\ell n[1-p(j)]\}$$

$$\equiv - \sum_{j=1}^{J} R(j) \, S(p(j))/k \quad . \tag{2.16}$$

Here $S(p(j))$, the Shannon entropy associated with $p(j)$, is a function only of the $p(j)$ since the $R(j)$'s are fixed.

The subsidiary conditions here consist of the requirements that the sum of the mean numbers of occupations,

$$\langle N \rangle = \sum_{j=1}^{J} \langle N(j) \rangle = \sum_{j=1}^{J} R(j)p(j) \quad , \tag{2.17}$$

and the sum of the mean number of occupations multiplied by the level energy of the respective assembly,

$$\langle E \rangle = \sum_{j=1}^{J} \langle N(j) \rangle \, E(j) = \sum_{j=1}^{J} E(j)R(j)p(j) \quad , \tag{2.18}$$

and both constants. It is straightforward then to extremize

$$F \equiv \{ \ell n \Lambda_R(<\underset{\sim}{N}>, \underset{\sim}{p}) + \alpha<N> + \beta<E> \} \qquad , \tag{2.19}$$

where α, β are Lagrange multipliers which turn out to have their usual mean-ings, namely, $\beta=1/kT$ and $\alpha=-\beta\mu$ with μ the chemical potential and T the abso-lute temperature. The extremum condition $\delta F/\delta p(j)=0$ leads to the extremum occupation factor which will be denoted by $f(j)$.

$$f(j) = (1+\exp[\alpha+\beta E(j)])^{-1} \tag{2.20}$$

This is of course the Fermi-Dirac occupation factor. Further it should be noted that

$$(\delta^2 F/\delta p(j)^2)_{p(j)=f(j)} = R(j)e^{\alpha+\beta E(j)}(e^{\alpha+\beta E(j)}+1)^2 > 0 \tag{2.21}$$

so that the Fermi-Dirac occupation factor minimizes F.

From Eq. (2.16), it is clear that the minimization principle for F is related to a maximization of the Shannon entropy of the underlying collection of binomial assemblies. This relationship will be discussed further in sec-tion V below.

It should also be pointed out that while the weight functions were not involved in the extremum principle, the entire probability functions were employed in establishing the relation between mean value numbers and occupa-tion factors. Thus all the quantities that enter into the binomial assem-blies enter into the present approach.

As a final observation in this section, it may be noted that passage to continuous energy spectrum is straightforward. All that is required is to interpret R(j) as the number of states in the sheet between energies E(j) and E(j)+dE(j).

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III. Negative Binomial Assemblies and Bose-Einstein Statistics

The Bose-Einstein occupation factor may be derived from negative binomial assemblies in a manner similar to the one used for Fermi-Dirac statistics in the previous section. However, the derivation does introduce an interesting subtlety in the definition of the occupation factor.

A negative binomial assembly consists of all possible distribution generated in the expansion of

$$p^R(1-q)^{-R} = 1 \qquad (3.1)$$

where R is the number of successful trials. A typical term in the expansion, say the Nth term, provides that probability function that there will be R successes at the (R+N))th trial

$$\bar{F}_R(N,p) = \binom{R+N-1}{N} p^R q^N \quad . \qquad (3.2)$$

The mean value of the number of trials beyond R necessary to achieve R successes is

$$\langle N \rangle = R(q/p) \qquad (3.3)$$

$\langle N \rangle$ is just the mean number of failures that occur along with R successes. Although the range of N in taking the mean value here is $0 \leq N \leq \infty$, this does not represent a requirement that N be large, only that it may be large. The actual specification of particle number is introduced through a subsidiary constraint condition.

Again if R is identified as the number of cells, then $\langle N \rangle$ may be viewed as the mean number of occupations in the R cells. The order of the failures is immaterial and their number is not limited so that their properties coincide with Bose-Einstein occupations. However in this case

$$\bar{p} = q/p \qquad (3.4)$$

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must be identified as the occupation factor. Note that $0<\bar{p}<\infty$ since $0<p<1$.
Equation (3.2) is readily rewritten in terms of $\bar{p}$, namely

$$\bar{F}_R(N,\bar{p}) = \binom{R+N-1}{N} \left(\frac{1}{1+\bar{p}}\right)^{R+N} \bar{p}^{\,N} \tag{3.5}$$

The combinatorial factor on the right hand side is the one that enters in the traditional treatment of Bose-Einstein statistics but is here the weight function.

$$\bar{W}_R(N) \equiv \frac{(R+N-1)!}{(R-1)!N!} \tag{3.6}$$

The remaining factor is the corresponding <u>load function</u>

$$\bar{\Lambda}_R(N,p) \equiv \left(\frac{1}{1+\bar{p}}\right)^{R+N} \bar{p}^{\,N} \tag{3.7}$$

Equations (3.3) and (3.4) may be used to express $\ln\bar{\Lambda}_R(<N>,\bar{p})$ in terms of $\bar{S}(\bar{p})$, the analog of the Shannon entropy of the occupation factor $\bar{p}$. $\bar{S}(\bar{p})$ is only an analog since $\bar{p}$ is an occupation factor rather than a probability.

$$\ln\bar{\Lambda}_R(<N>,\bar{p}) = R[\bar{p}\ln\bar{p}-(1+\bar{p})\ln(1+\bar{p})]\equiv-R\bar{S}(p) \tag{3.8}$$

In a manner completely analogous to that of the previous section, consideration of a set of negative binomial assemblies leads to the probability of $\underset{\sim}{N}$ occupations in $\underset{\sim}{R}$ cells

$$\bar{F}_{\underset{\sim}{R}}(\underset{\sim}{N},\underset{\sim}{\bar{p}}) = \bar{W}_{\underset{\sim}{R}}(\underset{\sim}{N})\bar{\Lambda}_{\underset{\sim}{R}}(\underset{\sim}{N},\underset{\sim}{\bar{p}}) \tag{3.9}$$

Here

$$\bar{W}_{\underset{\sim}{R}}(N) \equiv \prod_{j=1}^{J} \bar{W}_{R(j)}(N(j)) \tag{3.10}$$

The procedure is here to extremize

$$\bar{F} \equiv \{\ln\bar{\Lambda}_{\underset{\sim}{R}}(<\underset{\sim}{N}>,\underset{\sim}{\bar{p}}) + \alpha<N> + \beta<E>\} \tag{3.12}$$

where the constraints Eqs. (2.17) and (2.18) here have the same form but with $\bar{p}(j)$ replacing $p(j)$. The extremum occupation factor which will be denoted by $b(j)$ is just the Bose-Einstein occupation factor.

$$b(j) = [exp(\alpha+\beta E(j))-1]^{-1} \qquad (3.13)$$

Again this occupation factor corresponds to a minimum of $\bar{F}$ or a maximization of the Shannon entropy of the underlying collection of negative binomial assemblies. Treatment of a continuous energy spectrum can be handled in the same way as in section II.

IV. Poisson Assemblies and Maxwell-Boltzmann Statistics

Maxwell-Boltzmann statistics can be obtained as a high energy limit of either Fermi-Dirac or Bose-Einstein statistics. Alternatively one can obtain the Maxwell-Boltzmann occupation factor by considerations completely analogous to those of the previous two sections for the Poisson limit of binomial (and negative binomial) assemblies. Such a limit holds when all $R(j)$ are large and all $p(j)$ (or $\bar{p}(j)$) are small. In this limit, the analogs of Eqs. (2.14) and (2.15) (or Eqs. (3.10) and (3.11) become

$$W_R^P(\underset{\sim}{N}) = \prod_{j=1}^{J} (R(j)^{N(j)}/N(j)! \qquad (4.1)$$

$$\Lambda^P_R(\underset{\sim}{N})\underset{\sim}{m}) = \prod_{j=1}^{J} m(j)^{N(j)} e^{-R(j)m(j)} \qquad (4.2)$$

where $m(j)$ is either $p(j)$ or $\bar{p}(j)$. It may be noted that such weight and load functions are also immediately obtained from assembly frequency functions obtained from expansion of the identity

$$e^{-Rm} e^{Rm} = 1 \qquad (4.3)$$

In any event, minimzation of $\ln\Lambda^P_R(<\underset{\sim}{N}>,\underset{\sim}{m})$ subject to subsidiary conditions Eqs. (2.17) and (2.18) with $m(j)$ identified as the occupation factor yields the Maxwell-Boltzmann occupation factor.

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However, it may be observed that the weight function in Eq. (4.1) does not coincide exactly with the usual combinatorial term that arises in the discussion of Maxwell-Boltzmann statistics. Namely it lacks a factor of $N!$, where N is the total number of particles. Such a factor can readily be inserted in the weight function if its inverse is inserted in the load function. The important point is that such a factor does not enter into the extremum procedure and, in this sense, is a gauge factor in the determination of extremum occupation factors. Such a gauge factor could also have been introduced in the assembly collection weight and load functions of the previous sections without changing the results of those sections.

The fact that formalisms used to describe various types of particle statistics can be made to coincide in some limit does not mean that the particles whose statistics are being described coincide themselves. The statistics may be related but the particles retain their particular symmetry properties and their distinguishability or indistinguishability.

V.   Concluding Remarks

The present derivation of Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann occupation factors is based on a starting point in which both occupation possibilities and occupation configurations enter. Occupation possibilities are represented by the weight functions, and occupation configurations are represented by the load functions. The logarithm of the load function has been shown to be related to the negative of the Shannon entropy (or its analog) of these configurations. Application of a minimum principle to the logarithm of the load functions yields the usual results for particle statistics without identification of most probable values with mean values or the invocation of a large number approximation incorporated in Stirling's approximation. The present approach therefore seems to be more sound fundamentally.

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However, the fact that the traditional combinatorial approaches yield the same result is no accident but instead reflects a relationship between respective weight and load functions. The logarithm of a weight function provides a combinatorial entropy whereas the logarithm of a load function provides the negative of a configurational Shannon entropy. Thus an extremum principle on one is the complement of the other. Since the present approach employs a minimum principle for the negative of the Shannon entropy (or its analog), both approaches can be viewed as employing maximum entropy principles. However, it may be more appropriate to maintain focus on the negative entropy aspect and a minimum principle. Indeed one can interpret a set of particles organized with a specific statistics to be a manifestation of local order that should be characterized by a negative entropy contribution. Overall maximum disorder or entropy would then be achieved by a minimization of the negative entropy contribution.

Thus the present approach not only uses mean values rather than most probable values and relaxes the requirement for large total number of particles, but it also allows one to view the distribution of particles according to a particular occupation statistics to be an ordering process. All these features seem to be advantageous.

VI. Acknowledgment

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